Performance Assessment Challenges and Model Abstraction

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Disposal of long-lived radionuclides requires effective containment for 1,000 to 10,000 years or more, e.g.,

- Tank closures, saltstone
- Solid waste disposal
- D&D

However assumed performance beyond ~500 years requires explicit justification, e.g., NUREG-1573

- "Engineered barriers can . . . be assumed to have physically degraded after 500 years"
- "For timeframes longer than 500 years . . . credit . . . may be taken for the long-term provided the applicant provides suitable information and justification"
Engineered barriers and waste forms introduce significant modeling challenges:

- Reactive chemistry (grout and concrete)
- Evolution of physical and chemical properties over long time periods
- Highly contrasting material properties and fine geometric features (liners and fast flow paths)
Significant uncertainties

– Scenarios / conceptual models
– Closure state
– Exposure conditions
– Material properties and evolution

Uncertainties must be reduced and/or managed

– Experimental measurement
– Field validation
– Sensitivity analysis and uncertainty quantification
– Compliance margin

Features
Events
Processes

Many modeling cases
PA Challenges: Ambiguous Objectives

Period of Performance?

– DOE Order 435.1 → 1,000 yrs
– NRC guidance → 10,000 yrs

“Reasonable” expectation / assurance?

– Subjective criterion
– Role of behavior beyond period of performance

More modeling cases
Savannah River H-Tank Farm example

Vadose zone flow
- 4000 simulations = 5 scenarios · 20 tanks/srcs · 40 flow periods

Vadose zone transport
- Base case: 3200 runs = 40 tanks/srcs · 80 species
- Alternative cases: 1000 runs = 4 cases · 25 srcs · 10 species
- Sensitivity cases: 1000 runs = 10 scenarios · 10 srcs · 10 species
- Total: 5200 simulations

Aquifer transport
- 5200 simulations

Total = 14,400 simulations
PA Challenges: Schedule Constraints

Performance Assessment
- Months to one year

Revisions
- Weeks to months

Comment response
- Days to weeks

Modeling efficiency
Higher fidelity models for separate effects/phenomena and/or very-near field

- Cementitious material degradation
- Corrosion
- Reactive chemistry

System models for deterministic and limited sensitivity analysis

- Vadose zone / near-field
- Aquifer / far-field

Abstracted system model for sensitivity analysis and uncertainty quantification
Model abstraction required for efficiency

- Dimensionality: 3D → 2D → 1D
- Properties → fcn(time)
- Etc.

Savannah River H-Tank Farm example
Model integration

- Phenomena
- Regions
- Varying fidelity / abstraction
- Benchmarking
Higher fidelity models for simulating transport and degradation phenomena in cementitious materials

- Primary, secondary, and trace species transport
- External Sulfate Attack (~FY11)
- Carbonation (~FY12)
- Fractured materials (~FY13)

Experimental data

- Property measurements
- Validation data

Probabilistic framework

- Integration with GoldSim (www.goldsim.com)
Conceptual engagement through

- Source-term or boundary condition in near-field
  - for example, radionuclide release from waste form or through barrier
- Material property variations in space and time
  - for example, permeability
- Development of abstracted models

Software engagement through

- GoldSim interface
- Data files (for example, species flux as a function of time)
Example: CBP Source Term

ASCEM-CBP Joint Demonstration

- Relevant for estimating HLW tank system durability and radionuclide retention for
  - Performance assessments (PAs) as part of HLW tank closure
  - Tank integrity for continued use of single shell tanks at Hanford

- Primary phenomena:
  - Concrete carbonation (① & ②)
  - Steel liner corrosion (③)
  - Grout oxidation (④ & ⑤)
  - Contaminant diffusion (⑥)
  - Advective flux of water (⑦)

- ASCEM to simulate far-field to predict nominal flow (⑦)
- CBP to simulate near-field to model tank integrity, leaching, carbonation, corrosion, oxidation, diffusion and radionuclide release (①—⑥)
ASCEM-CBP Joint Demonstration

1. ASCEM far-field flow simulation
   - Flow field (CBP boundary condition)

2. CBP near-field simulation
   - Contaminant leach rate (ASCEM source term)

3. ASCEM far-field transport simulation
   - Contaminant flux to water table
Example: Effective Property

Approach:

• **STADIUM®** code used to predict formation of ettringite (coupled chemistry and transport analysis of major dissolved and solid species)

• **Simple damage model**
  – Ettringite = physical damage (e.g. cracking, spalling)
  – Transport properties not affected by ettringite front

• **Effective hydraulic properties by averaging**
Abstraction:

- Ettringite formation controlled by reaction capacity of concrete, $R$, and diffusion to front
  
  \[ R \frac{dx}{dt} = \frac{nD_e c}{x} \]
  
  - Reactant consumption rate
  - Reactant delivery rate

- Analytic solution for ettringite front
  
  \[ x = \left[ \frac{2nD_e c t}{R} \right]^{1/2} \]
Calibration of reaction capacity to STADIUM®:
Example: Effective Property

Effective Hydraulic Conductivity:

- Vault 2 wall
- Vault 2 floor
- Vault 2 roof

Elapsed Time (yr)
Effective Conductivity (cm/s)

Compliance period
Summary

• CBP data and software are designed to address PA challenges arising from
  – Long time frames
  – Cementitious material degradation
  – Uncertainty
  – Computing and schedule limitations

• CBP software tools can engage the PA process in multiple ways
  – Provide higher fidelity models for particular phenomena
  – Support model abstraction

• CBP tools are ‘GoldSim-ready’